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Atomization of liquid fuels is studied by numerical simulations. The Navier-Stokes equations are solved by a finite difference/front tracking technique that allows resolution of inertial and viscous forces as well as the inclusion of surface tension at the deformable boundary between the fuel and the air. The secondary breakup of drops has been examined by extensive axisymmetric simulation of four systems: Impulsive and gradual disturbances for two different density ratios (1.15 and 10). At low density ratios. the density disappears as an independent control parameter and we have shown that the low density results apply to density ratios as high as two if we rescale time using the Boussinesq approximation. In addition to full simulations where the Navier-Stokes equations are solved, a few inviscid simulations have also been done for the small density ratio case to isolate the effect of viscosity. The breakup of a planar interface has been examined. The presence of surface tension leads to the generation of fingers of interpenetrating fluids. In the limit of a small density ratio the evolution is symmetric, but for large density stratification the large amplitude stage consists of narrow fingers of the denser fluid penetrating into the less denser one. The dependency of the density difference is explained in terms of the advection of interfacial vorticity by the density weighted mean velocity.

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COMPUTATIONAL INVESTIGATION OF ATOMIZATION

AFOSR-contract F49620-96-1-0356

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Atomization of liquid fuels is studied by numerical simulations. The Navier-Stokes equations are solved by a finite difference/front tracking technique that allows resolution of inertial and viscous forces as well as the inclusion of surface tension at the deformable boundary between the fuel and the air. The secondary breakup of drops has been examined by extensive axisymmetric simulation of four systems: Impulsive and gradual disturbances for two different density ratios (1.15 and 10). At low density ratios, the density disappears as an independent control parameter and we have shown that the low density results apply to density ratios as high as two if we rescale time using the Boussinesq approximation. In addition to full simulations where the Navier-Stokes equations are solved, a few inviscid simulations have also been done for the small density ratio case to isolate the effect of viscosity. The breakup of a planar interface has been examined. The presence of surface tension leads to the generation of fingers of interpenetrating fluids. In the limit of a small density ratio the evolution is symmetric, but for large density stratification the large amplitude stage consists of narrow fingers of the denser fluid penetrating into the less denser one. The dependency of the density difference is explained in terms of the advection of interfacial vorticity by the density weighted mean velocity.

Objectives

Numerical simulations of the deformations and breakup of drops are being done, for both shock generated disturbances as well as gradual disturbances, where inertial and viscous effects for both the drop and the ambient gas as well as surface tension effects are fully accounted for. The simulations will help determine where in parameter space the various breakup modes take place, how long breakup takes, and what the resulting drop size distribution is. The goal of the investigation is to provide results that extend and complement experimental investigations, and lead to better engineering models of drops in sprays. Simulations are also being done on the breakup of jets to determine the size of the primary drops.

These computations are made possible by a recently developed numerical technique that has been used already for a number of multifluid problems. The method incorporates an explicit tracking of the drop surface with a finite difference method for the full Navier-Stokes equations for the drop and the ambient gas. Arbitrary differences in density and viscosity are possible, large surface deformations are allowed and surface tension is fully accounted for. For problems with mass and heat transfer, conservation equations for mass and energy are solved also. The technique has been used for two-dimensional, axisymmetric, and fully three-dimensional problems and validated extensively by comparisons with analytical solutions for simple cases, other numerical studies, grid refinement, and experiments.

Status of Effort:

To examine the breakup of drops as the density difference becomes smaller, extensive axisymmetric simulation of four systems have been done: Impulsive and gradual disturbances for two different density ratios (1.15 and 10). At low density ratios, the density disappears as an independent control parameter and we have shown that the low density results apply to density ratios as high as two if the time is rescaled using the Boussinesq approximation. In addition to full simulations where the Navier-Stokes equations are solved, a few inviscid simulations have also been done for the small density ratio case to isolate the effect of viscosity.

A series of two-dimensional simulations of the breakup of a planar interface have been done and the evolution examined as a function of the density ratio of the fluids, the Reynolds number in each fluid, and the Weber number.

Accomplishments/New Findings:

The breakup of the drops is governed by four nondimensional numbers. In addition to the density and viscosity ratio, the ratio of inertia to surface tension is described by an Eötvos number for gradual disturbances and a Weber number for impulsive acceleration. The effect of viscosity is described by the Ohnsorge number (the ratio of the viscous force to the surface tension). Our simulations have now resulted in a fairly complete picture of the evolution at small density ratios. For small Eotvos and Weber numbers the drops remain spherical in all cases, independently of the Ohnsorge number and density and viscosity ratio. If the Ohnsorge number is low, the deformations of the drop depend only on the Eotvos/Weber number (and the density ratio). As the Eotvos/Weber number is increased, the drops deform into a disk-like shape due to high pressure at the fore and aft stagnation points and low pressure around the equator. For gradual disturbances this results in a steady state motion where the work done by the constant acceleration is dissipated by the drag on the drop, but for impulsive acceleration the drop oscillates. Increasing the

Eotvos/Weber number further results in a continuing deformation where most of the drop fluid ends up in a taurus connected by a thin film. For moderate Eotvos/Weber numbers, the initial momentum of the drops is relatively low and once the taurus is formed, the rim moves faster than the film for drops with gradual disturbances. The film "bulges" back and experimentally is seen that this bag eventually breaks. The simulations have shown that the bag break-up mode is a viscous phenomenon, due to flow separation at the rim of the drops and the formation of a wake, and therefore not seen in inviscid computation. For drops subject to an impulsive acceleration, the formation of a backward facing bag is only seen for the higher density ratios. Bag breakup requires a driving force that acts stronger on the drop than on the surrounding fluid and for impulsively accelerated drops this driving force is the fluid inertia. As the density difference becomes small, the difference between the drop and the fluid inertia vanishes and the low density ratio drops simply stop and surface tension pulls them back into a spherical shape. Experimentally, bag breakup is commonly observed, but the density ratio is larger than simulated here. Increasing the Eotvos or the Weber further, results in a different mode of breakup that also depends on the density ratio. For low density ratios, the fluid initially still ends up in the rim of the drop, but the initial momentum is now sufficiently large that the ambient fluid moves the film faster than the taurus, leading to a bag that extends forward of the drop. For higher density ratios, not all the fluid moves to the rim resulting in a taurus connected to the rest of the drop by a thin sheet. As this sheet is pulled from the drop, the fluid is drained from the drop. As the driving force is increased the size of the rim is reduced and for very high Eotvos/Weber numbers, small drops are pulled from the rim. Examination of the dynamic of the vorticity generated at the drop surface and the effect of surface tension and a large density difference have been used to explain some of the different trends observed. The vortex dynamics suggests that the shear breakup mode where fluid is stripped from the rim of the drop by an essentially inviscid effects. Simulations show, for example that unlike the bag breakup case, separation does generally not take place. We have, however, not yet done inviscid simulations for large density ratios to confirm that this is the case. In the transition between a bag breakup mode and shear breakup, we have found drops that oscillate in a chaotic manner. Such transition phenomena have been seen experimentally for higher density ratios.

In addition to the Ohnsorge number effect, where the boundary between breakup modes is shifted to higher Eotvos/Weber numbers as viscous effects become more important, the fluid and drop viscosity can change the drop shape during breakup if the Ohnsorge number is high enough. High viscosities can, for example lead to skirted drops at low density ratios, where thin fluid skirts are pulled from the rim of the fluid, in a way similar to the shear breakup seen for higher density ratios.

Figure 1 shows the breakup of several impulsively accelerated drops for a density ratio of ten and different Weber numbers. Other parameters are given in the figure. Each column is a different case and the initial spherical drop is shown at the top of each column. Notice that the nondimensional times have been selected differently for each sequence. Initially, when the drop has been given a velocity relative to the surrounding fluid, it becomes flatter. For low Weber numbers the drops do not break up, but as the Weber number is increased, they start to oscillate and the amplitude of the oscillations increases, eventually leading to bag breakup. At even higher Weber number, shear breakup takes place and for an infinitely high Weber number (zero surface tension) small drops are torn from the edge of the drop. While the resolution is not sufficient to fully resolve these drops, the evolution is similar to what is observed experimentally.

The simulations have been used to generate "break-up" maps for low density ratios and it is found that the general character of those maps agrees with what has been found experimentally at larger density ratios. At low Ohnsorge numbers the transition between the

various modes depends only on the density ratio and the Eotvos number, but a high Ohnsorge number will move the transition to a higher Eotvos number. However, there are some fundamental differences like the absence of a bag breakup for low density impulsive drops.

In the present simulations, the actual breakup of the drops has not been followed. While it is relatively simple to allow interfaces to break, the length scales involved are too small to resolve in a simulation that also follows the rest of the drop. While the current methodology has been used to follow the draining of a thin film to the point when it breaks, in simulations of colliding drops, it is likely to be more practical to model the actual breakup separately. A techniques to estimate the distribution of drop sizes after breakup based on local applications of the conservation of mass and surface tension energy is currently under development. The drop size distribution is nearly always bimodal for small density ratios, with small drops coming from the bag and the rest of the drop forming larger drops. It is, however, already clear that in situations where secondary breakup takes place, the smallest drop sizes are not generally obtained by making the primary drops as small as possible. Since larger primary drops can result in smaller drop sizes after secondary breakup, it is possible that there is an optimum size of the primary drops for a given acceleration.

A series of two-dimensional simulations of the breakup of a planar interface have been done. The evolution is determined by the density ratio of the fluids, the Reynolds number in each fluid, and the Weber number. Unlike the Kelvin-Helmholtz instability for miscible fluids, where the sheared interface evolves into well defined concentrate vortices if the Reynolds number is high enough, the presence of surface tension leads to the generation of fingers of interpenetrating fluids. In the limit of a small density ratio the evolution is symmetric, but for large density stratification the large amplitude stage consists of narrow fingers of the denser fluid penetrating into the less denser one. The dependency of the density difference is explained in terms of the advection of interfacial vorticity by the density weighted mean velocity. Even though the simulations are confined to only the two-dimensional aspects of the problem, it is found that the fingers can break up into isolated drops. While the initial growth rate is well predicted by inviscid theory, once the Reynolds numbers are sufficiently high, the large amplitude behavior is strongly affected by viscosity and the mode that eventually leads to fingers is longer than the most unstable one.

During the next year, the focus of the investigation will be two fold:

- Further quantification of the results obtained so far, including estimated of drop sizes and the time it takes a drop to disintegrate and the completion of papers describing the axisymmetric drop break-up and the break-up of a two-dimensional interface.
- Three-dimensional aspects of both the drops and the jets breakup, again, focusing on the ultimate size of the drops after breakup.

Personnel Supported:

Gretar Tryggvason, Professor
Jaehoon Han, Graduate Student, currently a postdoctoral fellow
Saeed Mortazavi, Postdoctoral Fellow (part time)

Publications:

G. Tryggvason & S.O. Unverdi. The Shear Breakup of an Immiscible Fluid Interface. Proceedings of the C.S. Yih Memorial Symposium. Ed. W. Shyy. Cambridge University Press, 1999.

G. Tryggvason, A. Esmaeeli, S. Mortazavi, J. Han, and S. Homma. Computations of Multiphase Flows by a Finite Difference/Front Tracking Method. II Applications. In: 29th Computational Fluid Dynamics. Lecture Series 1998-03. Von Karman Institute for Fluid Dynamics.

J. Han. *Numerical Studies of Drop Motion in Axisymmetric Geometry.* Ph. D. Dissertation. University of Michigan, 1998.

W. Tauber, S. O. Unverdi, and G, Tryggvason. The shear breakup of fluid interfaces. Proceedings of the ASME Summer Meeting of the Fluids Division, Washington DC, 1998.

G. Tryggvason, B. Bunner, A. Esmaeeli, and S. Mortazavi. Direct simulations of dispersed flow. Proceedings of the Third International Conference on Multiphase Flow. Lyon, France, June 8-12, 1998.

Journal articles are in preparation

Interactions/Transitions:

(a) Since September 1, last year, I have discussed various aspects of the present work in the following presentations:

G. Tryggvason. Seminar at UCSB, Chemical Engineering. 11/21/97

G. Tryggvason. Seminar at the University of Arizona, 1/29/98

G. Tryggvason. Seminar at NASA Lewis Research Center, 3/10/98

J. Han & G. Tryggvason. Air induced breakup of drops. 50th Meeting of the American Physical Society, Div of Fluid Dynamics, Nov. 23-24. San Francisco, CA. Abstracts in Bull. Amer. Phys. Soc

G. Tryggvason, B. Bunner, S. Mortazavi, & A. Esmaeeli "Direct Numerical Simulations of Dispersed Multiphase Flows. 11th Japanese Symposium on CFD. Tokyo, Japan. December, 1997. Invited Opening Lecture. (See also publications)

G. Tryggvason. Computations of Multiphase Flows by a Finite Difference/Front Tracking Method. Lecture Series 1998-03. Von Karman Institute for Fluid Dynamics. Belgium. February 23-27, 1998. (See also publications)

G. Tryggvason, B. Bunner, A. Esmaeeli, and S. Mortazavi. Direct simulations of dispersed flow. Third International Conference on Multiphase Flow. Lyon, France, June 8-12, 1998. (See also publications)

W. Tauber, S. O. Unverdi, and G, Tryggvason. The shear breakup of fluid interfaces. ASME Summer Meeting of the Fluids Division, Washington DC, 1998. (See also publications)

G. Tryggvason & S.O. Unverdi. The Shear Breakup of an Immiscible Fluid Interface. 13th U.S. National Congress of Applied Mechanics. Gainesville, FL, June 21-26, 1998. (See also publications)

(b) I consult regularly for Ford Motor Company, GRI, and the Fermi II Nuclear Power Plant.

(c) The numerical method used in this investigation is currently being used by Dr. E. Steinthorsson at Parker Hannifin Corporation to investigate the formation of a fluid sheet from a SIMPLEX nozzle and the subsequent breakup of the sheet into drops.

New discoveries, inventions or patents:

None

Honors/Awards:

Invited to give the opening lecture for the 11 Japanese Symposium on CFD. Tokyo, Japan. December, 1997.

Invited to give a series of three lectures at the von Karman Institute

Impulsive acceleration

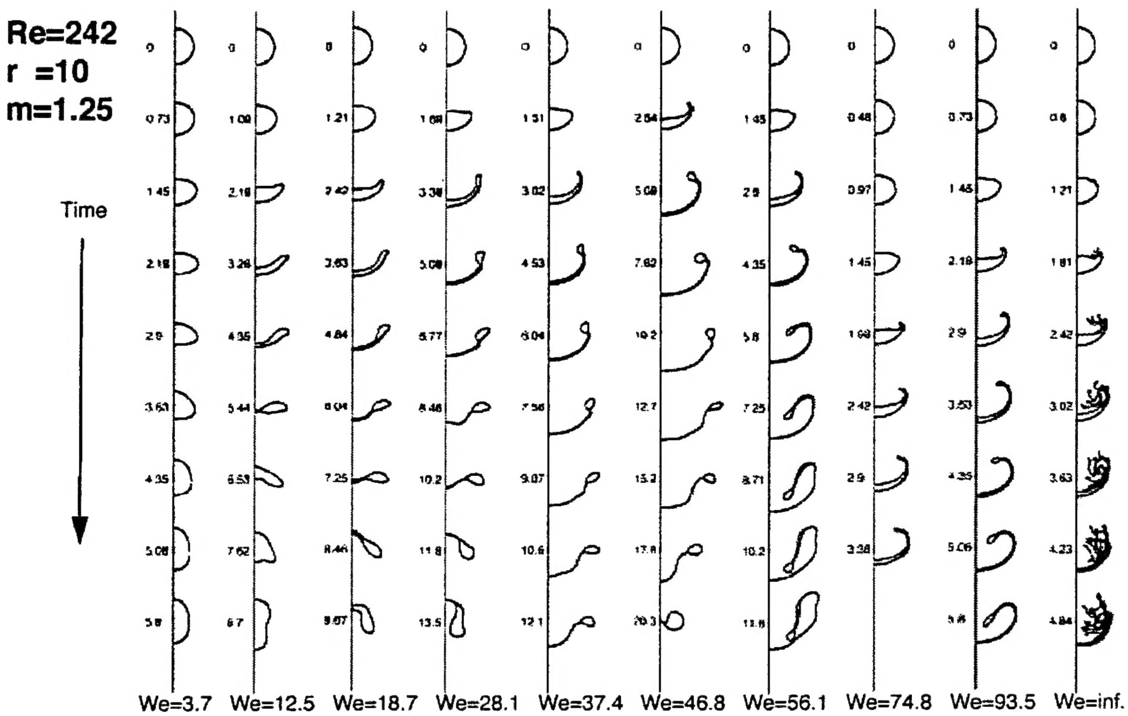

Figure 1. Several computations of the breakup of impulsively accelerated drops.

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PI DATA

Name (Last, First, MI): Tryggvason, Gretar

Institution: University of Michigan

Contract/Grant No.: FA9620-96-0356

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PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT

NOTE: List names in the following format: Last Name, First Name, MI

Include: Articles in peer reviewed publications, journals, book chapters, and editorships of books.

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